

## **IMPACT OF DATA UNCERTAINTY ON IDENTIFYING LEAKAGE PATHWAYS IN CO<sub>2</sub> GEOLOGIC STORAGE SYSTEMS AND ESTIMATING THEIR HYDROGEOLOGICAL PROPERTIES BY INVERSE MODELING**

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### **ABSTRACT**

For successful risk management of large-scale geologic carbon storage (GCS), it is crucial to detect leakage of brine and/or CO<sub>2</sub> from a storage reservoir through unknown leakage pathways (e.g., abandoned wells and faults) as early as possible, and to determine the leak's impact on the environment. We are currently developing a monitoring and inverse modeling framework for early leakage detection, which uses anomalies in monitoring data on pressure-driven processes—such as pressure measurements from monitoring wells within and above the storage reservoir, as well as surface-deformation InSAR data—as early signals of brine and/or CO<sub>2</sub> leakage through unknown leakage pathways. In a study of idealized GCS scenarios, we have demonstrated the strong sensitivity of pressure and deformation anomalies (i.e., the differences between leakage and no-leakage scenarios) to the location and permeability of potential leakage pathways, and we have successfully detected leakage pathways and calibrated their permeabilities using the approach of modeling and jointly inverting pressure and surface deformation data. However, noise in monitoring data (large random errors or non-normal errors) and drift in pressure transducers (systematic errors) may lower detectability (due to the increased uncertainty they cause), and even lead to failure of leakage detection and parameter estimation. In addition, uncertainties in measured or presumably known hydrogeological properties of the storage system may also increase the difficulty of identifying leakage pathways.

Here, we use iTOUGH2 to examine the effect of various data uncertainties on the accuracy of

detection and estimation, and discuss strategies for enhancing detectability and reducing the impact of those uncertainties.

### **INTRODUCTION**

For geologic carbon sequestration (GCS) to have a sizable effect on mitigating climate change, large volumes of CO<sub>2</sub> must be injected into subsurface reservoirs (Benson and Cole, 2008). However, large-scale CO<sub>2</sub> injection may result in a substantial increase in pressure within the storage formation and heighten the potential risks of GCS (Zhou et al., 2010). Brine or CO<sub>2</sub> may leak through unknown high-permeability leakage pathways (e.g., abandoned wells and faults) within the area of influence. In addition, increased pore pressure in the storage reservoir could induce geomechanical alteration of the reservoir and its surroundings, e.g., creating new fractures or reactivating larger faults (Rutqvist, 2012). If these changes occur in the cap rock or overburden, they could become new leakage pathways for brine or CO<sub>2</sub>, potentially resulting in localized deformation (in addition to injection-induced deformation). If such leakage events cannot be properly assessed, GCS might cause undesirable environmental and safety consequences, and these events might ultimately prevent future deployment of GCS. Therefore, it is essential to the success of GCS for us to have the ability to detect brine or CO<sub>2</sub> leakage from the storage reservoir through high-permeability pathways, predict potential risk profiles, and manage the risks as early as possible.

We are currently developing a monitoring and inverse modeling framework for early leakage detection, using multiple complementary data sources, such as pressure buildups in monitoring

wells within and above the storage reservoir and surface-deformation data (e.g., Interferometric Synthetic Aperture Radar, InSAR). Within this framework, potential leakage pathways are identified and located as early as possible by inverse modeling of anomalies in monitoring data, and the time-dependent likelihoods of CO<sub>2</sub> leakage through the identified pathways are predicted using calibrated models. Unlike existing leakage-detection techniques, this framework will help with early detection and thereby allow time for risk mitigation and management in advance of actual CO<sub>2</sub> leakage.

In a recent study of idealized GCS scenarios (Jung et al., 2012), we demonstrated the strong sensitivity of pressure and deformation anomalies (i.e., the differences between leakage and no-leakage scenarios) to the location and permeability of potential leakage pathways, and we have successfully detected model leakage pathways and calibrated their permeabilities using the approach of modeling and jointly inverting pressure and surface deformation data. However, the monitoring data available in practical applications may not always be ideal, and such data will likely contain errors that may not automatically be accounted for in the calibrated model. For instance, noise in monitoring data (large random errors or non-normal errors) and instrument drift in pressure transducers (systematic errors) may increase uncertainties in parameter estimation and even lead to failure of leakage detection. In addition, hydrogeological properties obtained from other tests or sources and considered as known parameters may not be error-free, and these uncertainties in the hydrogeological properties of the storage system can increase the difficulty of identifying leakage pathways. Therefore, it is important to assess the impact of data uncertainty on identifying leakage pathways in GCS systems and estimating their hydrogeological properties by inverse modeling.

In this paper, we briefly introduce the concept of early leakage detection, discuss the sensitivity of pressure monitoring for leakage detection, and demonstrate the feasibility of identifying and estimating leakage pathways (and their hydrogeological properties) by inverse modeling in an idealized monitoring scenario. Then, we

examine the effect of various data uncertainties on the accuracy of detection and estimation. For simplicity here, we limit our discussion to using only pressure data from monitoring wells.

### **PRESSURE-BASED EARLY DETECTION FRAMEWORK FOR CO<sub>2</sub> LEAKAGE FROM STORAGE RESERVOIRS**

Our early leakage detection framework for GCS is based on the idea of (1) using the signals of fast-traveling pressure-buildup waves (caused by CO<sub>2</sub> injection into the storage reservoir) and pressure-induced surface deformation, and their signal anomalies associated with seal imperfections (e.g., leaky faults, fractures, abandoned wells) to locate, identify, and quantify these seal imperfections; (2) predicting the fronts of slower-migrating CO<sub>2</sub> plumes by flow modeling, with the locations and hydrologic properties of the detected seal imperfections accounted for; and (3) comparing the two time-evolving inverse- and forward-modeling processes to predict the time-dependent likelihood of CO<sub>2</sub> leakage through these features, and to guide mitigation measures to prevent leakage from happening if such likelihood exists.

The core of this approach is to jointly utilize fast-propagating pressure data and high-spatial-resolution surface deformation data to improve the detectability of leakage signals and reduce the uncertainties in locating leakage pathways. Time-dependent pressure buildups caused by CO<sub>2</sub> injection propagate much faster than the CO<sub>2</sub> plume migrates, and therefore the anomalies in observed pressure buildups, which are induced by brine leakage through leakage pathways, may also be revealed quickly. However, only a few monitoring wells may be available (if any), and they may not always be conveniently located close to leakage pathways, such that they could sensitively detect anomalies in pressure buildups. Therefore, surface deformation InSAR data, which can measure ground displacement on the order of centimeters or millimeters and provide dense spatial information on the scale of kilometers, might be able to add useful complementary information for detecting leakage pathways.

## METHODOLOGY

### Model Setup and Parameters

We consider a simplified conceptual model, which represents a storage system consisting of a target storage formation, a cap rock, and an overlying monitoring formation, as shown in Figure 1. The injection well (IW) is located at the center of the model domain [0 km, 0 km], and the leaky well (LW) is located 2 km away from the injection well [2 km, 0 km]. Resident brine is injected into the storage reservoir at a constant rate,  $Q = 5700 \text{ m}^3 \text{ day}^{-1}$ , and pressure perturbations arising from fluid injection and brine leakage are observed at monitoring wells. The radius of the injection, the leaky well, and the monitoring wells is 0.15 m. The effective permeability of the leaky well is  $k_L = 10^{-10} \text{ m}^2$ . The following properties are used as the formation parameters of the storage system: aquifer (storage and overlying formation) thickness of  $B = 60 \text{ m}$ , aquifer permeability of  $k = 10^{-13} \text{ m}^2$ , aquifer pore compressibility of  $\beta_p = 4.5 \times 10^{-10} \text{ Pa}^{-1}$ , aquitard (caprock formation) thickness of  $B' = 100 \text{ m}$ , aquitard permeability of  $k' = 10^{-18} \text{ m}^2$ , aquitard pore compressibility of  $\beta'_p = 9.0 \times 10^{-10} \text{ Pa}^{-1}$ , and water compressibility of  $\beta_w = 3.5 \times 10^{-10} \text{ Pa}^{-1}$ . Accordingly, the hydraulic conductivities of the aquifers and the aquitard are  $0.20 \text{ m day}^{-1}$  and  $0.20 \times 10^{-5} \text{ m day}^{-1}$ , respectively, assuming brine density of  $\rho = 1200 \text{ kg m}^{-3}$ , gravity acceleration of  $g = 9.8 \text{ m s}^{-2}$ , and water viscosity of  $\mu = 0.5 \times 10^{-3} \text{ Pa s}$ . The specific storativity of the aquifers is calculated using  $S_s = \phi \rho g (\beta_w + \beta_p) = 1.88 \times 10^{-6} \text{ m}^{-1}$ , where the aquifer's porosity is  $\phi = 0.2$ . The specific storativity of the aquitard is calculated using  $S'_s = \phi' \rho g (\beta_w + \beta'_p) = 1.47 \times 10^{-6} \text{ m}^{-1}$ , where the aquitard porosity is  $\phi' = 0.1$ . These formation parameters are based on previous studies on large-scale injection of  $\text{CO}_2$  (Birkholzer et al., 2009) and water (Zhou et al., 2009).

### Computational Methods

To calculate pressure buildups in the storage system, we use an efficient semi-analytical solution (Cihan et al., 2011), assuming single-phase water flow. This solution can calculate pressure perturbation and fluid flow that are induced by large-scale fluid injection in multilayer systems (e.g., multiple aquifers and

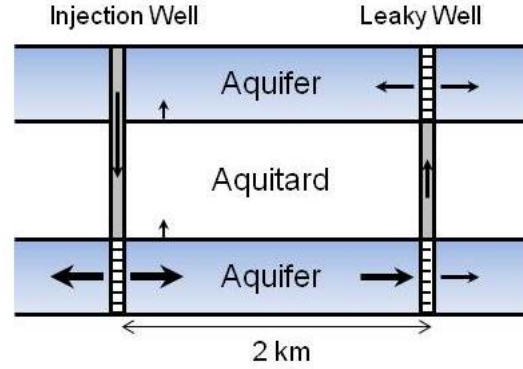


Figure 1. Schematics of a simplified storage system of a target storage reservoir, a caprock, and an overlying aquifer, with an injection well and a leaky well (2 km away).

alternating aquitards), combining the effect of diffuse leakage through aquitards and/or focused leakage through leaky wells. The fluid flow in the system is described by coupled one-dimensional horizontal flow in aquifers, vertical flow in aquitards, and Darcy-type vertical flow in leaky wells. Further details on this analytical solution can be found in Cihan et al. (2011).

For inverse modeling, we use iTOUGH2-PEST (Finsterle, 2011). iTOUGH2-PEST is an extended version of iTOUGH2, a computer program for parameter estimation, sensitivity analysis, and uncertainty propagation analysis (Finsterle, 2007), and uses the PEST protocol (Doherty, 2007, 2008) as a way to communicate between application models and iTOUGH2. iTOUGH2 was originally developed for use with the TOUGH2 forward simulator (Pruess, 1999). However, with the iTOUGH2-PEST module, iTOUGH2 can be used as a universal optimization code for non-TOUGH2 models.

### DETECTION OF PRESSURE ANOMALIES

Large volumes of  $\text{CO}_2$  injection into the storage formation may induce significant pressure buildups. Hydraulic communication between the storage and the overlying formation via diffuse leakage through the cap rock may also influence pressures in both formations. Such pressure perturbations in GCS systems can be simulated using appropriate models, e.g., Cihan et al. (2011). Therefore, for an idealized system with homogenous aquifers and aquitards, the difference between the measured pressures at

monitoring wells and the calculated values based on known hydrogeological properties of the storage system can be attributed to the leakage through unknown leakage pathways. The detectability of this leakage signal greatly depends on various formation parameters, as well as the effective permeability of the leakage pathways.

To determine how sensitively the pressure at monitoring wells changes in response to brine leakage through a leaky well, we compute the absolute difference of pressures measured with and without the presence of the leaky well ( $|h_w - h_{w0}| = \Delta h_{w-w0}$ ). While the sensitivity of the calculated  $\Delta h_{w-w0}$  to the parameters varied with time and space, the most influential parameter on the whole was found to be the permeability of the cap rock (Jung et al., 2012). We therefore present the result for three different values of aquitard permeability ( $k' = 10^{-19}$ ,  $10^{-18}$ , and  $10^{-17}$  m<sup>2</sup>).

Figure 2 shows the time-dependent contour lines of (a)  $\Delta h_{w-w0} = 1$  m and (b)  $\Delta h_{w-w0} = 0.1$  m in the overlying aquifer. Here, the  $\Delta h_{w-w0}$  values might be assumed to be the minimum pressure buildup to be considered as anomalies induced by high-permeability leakage pathways in different conditions. For instance,  $\Delta h_{w-w0} = 1$  m may be used as the detection limit when noises in monitoring data are rather large, and  $\Delta h_{w-w0} = 0.1$  m when noises are small. In both cases, the contour lines are centered around the leaky well located at [2 km, 0 km]. In other words,  $\Delta h_{w-w0}$  in Figs. 2a and 2b is higher than 1 m and 0.1 m, respectively, inside the contour line at each time. This means that the detectability of pressure anomalies at monitoring wells would be highly dependent on the location of a monitoring well relative to a leaky well.

Similarly, the time-dependent contour lines of  $\Delta h_{w-w0} = 0.1$  m in the overlying formation are shown in Fig. 3 for the case of  $k' = 10^{-17}$  m<sup>2</sup>. The area in which the anomalies can be detected increases with time, but the area is significantly smaller for the higher-permeability case ( $k' = 10^{-17}$  m<sup>2</sup>, Fig. 3) than that in the base case ( $k' = 10^{-18}$  m<sup>2</sup>, Fig. 2b), particularly for late times. An

important implication of this result is that early leakage detection is especially critical if the sealing layer has a relatively high permeability. Unless leakage is detected early enough at monitoring wells, it might be difficult to discern leakage signals induced by the presence of high-permeability conduits, such as faults and abandoned boreholes from those by a slow, diffuse process. That is, the accuracy of hydrogeologic parameters (e.g., the cap-rock permeability), which is usually determined by other survey techniques and assumed to be known, might have a large impact on parameter estimation using inverse modeling. (This effect is discussed later.) The difference between the lower-permeability case ( $k' = 10^{-19}$  m<sup>2</sup>) and the base case ( $k' = 10^{-18}$  m<sup>2</sup>) was relatively minor, implying diffuse leakage through the caprock is not substantial for the aquitard permeability of up to  $k' = 10^{-18}$  m<sup>2</sup>.

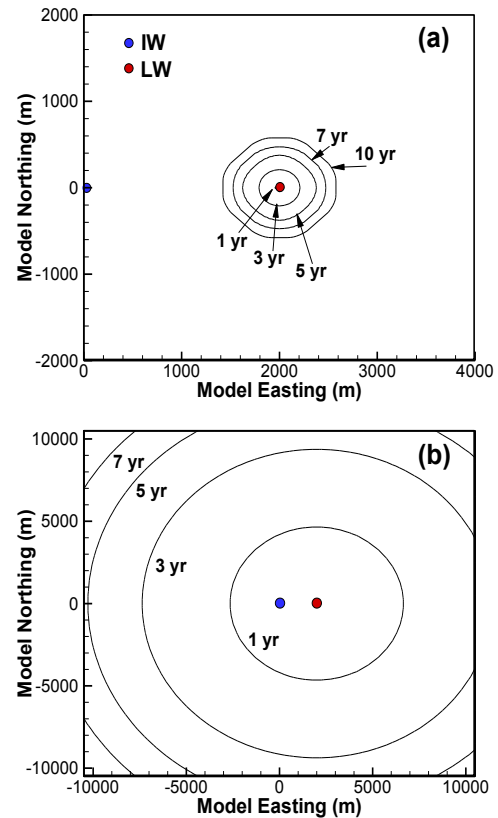


Figure 2. Time-dependent contour lines of (1)  $\Delta h_{w-w0} = 1$  m and (b)  $\Delta h_{w-w0} = 0.1$  m in the overlying formation for the base case of  $k' = 10^{-18}$  m<sup>2</sup>.

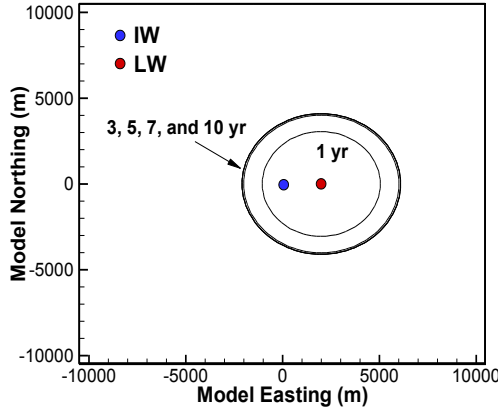


Figure 3. Time-dependent contour lines of  $\Delta h_{w-wo} = 0.1$  m in the overlying formation for the higher-permeability case of  $k' = 10^{-17} \text{ m}^2$ .

### **PARAMETER ESTIMATION: IDEALIZED MONITORING SCENARIO**

This section presents an idealized monitoring scenario and examines the ability of identifying/locating a leaky well using inverse modeling against pressure data, and calibrating the effective permeability. In addition to the injection well, two monitoring wells (MW1 and MW2) are available for pressure observation in both the storage and the overlying formation, and they are located at [1.5 km, 1.5 km] and [-1.5 km, 1.5 km], respectively. The pressure data collected from these monitoring wells contain only small amount of instrument measurement noise (zero-mean Gaussian noises with standard deviation of 0.0014 bar, which is twice that of the instrument resolution). Here, we assume that any natural background fluctuations due to atmospheric-pressure changes, earth tides, and ocean tides can be filtered out from the data. We use the pressure data measured at the monitoring wells in the storage and the overlying formation and at the injection well in the overlying formation, and test four different initial guesses of the leaky well location at  $[\pm 1 \text{ km}, \pm 1 \text{ km}]$  for estimating the leaky well location and permeability.

The match between the computed and the measured pressure buildups was excellent, and all the residuals appeared random (see Fig. 4). The location and effective permeability of the leaky well were also successfully estimated using iTOUGH2-PEST, regardless of the initial guesses away from the actual location. Since the

inversion accuracy could be affected by the configuration of available monitoring wells (Jung et al., 2012), we use the same setup in the following section to explore the effect of noise in data and model structure.

### **PARAMETER ESTIMATION: EFFECT OF RANDOM AND SYSTEMATIC ERRORS**

Various errors are introduced into the model and synthetic data (see Table 1) to examine their impact on parameter estimation: (1) the cap-rock permeability derived from other hydraulic tests is overestimated by 20% ( $k' = 1.2 \times 10^{-18} \text{ m}^2$ ), (2) the drift in the pressure transducer at MW1 in the overlying formation linearly increases over time (drift rate =  $0.001 \text{ m d}^{-1}$ ), and (3) the pressure measured in the storage formation exhibits pressure-dependent random fluctuations (zero-mean random noises with heterogeneous standard deviation, which increases up to 0.14 bar).

To enhance the fit between the measured and calculated pressures, we incrementally increased the number of parameters considered. At first, similar to the idealized monitoring case, only the location and permeability of the leaky well were estimated. In our second attempt, the permeability of the sealing caprock was included as one of the parameters to be estimated. In the third calibration, the drift rate of the pressure sensor at MW1 in the overlying formation was also parameterized and estimated along with the other parameters. Finally, heteroscedasticity in the monitoring data was also considered in the calibration.

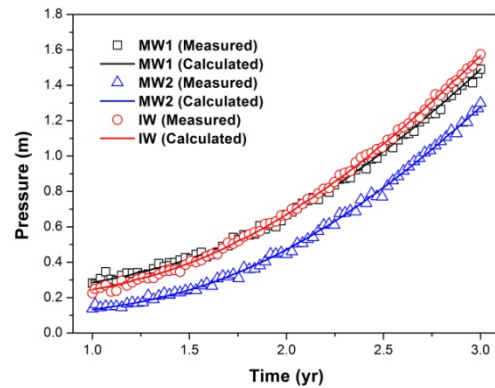


Figure 4. Comparison between the measured and calculated pressures in the overlying formation.

Table 1. Various random and systematic errors introduced into the model and the data.

Error Description	Error Type
• Wrong caprock permeability	Systematic modeling error
• Drift in MW1 pressure transducer in the overlying formation	Systematic measurement error
• Pressure-dependent measurement errors in the storage formation	Heteroscedastic random error

Figure 5 shows the measured against calculated pressures in the storage (SF) and the overlying formation (OF). The estimated parameters in each inversion are summarized in Table 2. As shown in Fig. 5a, when simply the location and permeability of the leaky well are calibrated, the residuals (the deviations from the unit-slope line) at MW2 and IW in the overlying formation are significantly large, indicating that the model failed to account for the true system, and that some systematic errors influenced the inversion results. The observation that the deviations were greater when the distance between the monitoring point and the leaky well was larger suggests that the initial value used for the aquitard permeability was erroneous.

In the second trial, the permeability of the caprock was parameterized and the fit was then significantly improved (see Fig. 5b). The standard deviation of the estimated parameters also largely decreased. However, even if the degree of deviation was a lot smaller than that in Fig. 5a, all the pressures calculated in the overlying formation still show systematic deviations, suggesting that a more refined model is required. Another interesting observation here is that the estimated leaky well location is almost identical with the location of MW1. If the errors in the model are not carefully analyzed, this erroneous estimate may result in biased conclusions (e.g., a leak in MW1 itself).

In the third inversion, the drift of pressure sensor in MW1 was included as one of the parameters estimated. The residuals of all the pressures measured in the overlying formation appeared

random (see Fig. 5c), and the estimated parameters were reasonably acceptable (see Table 2).

Based on the residual analysis, the residuals of the pressures measured in the storage formation also appeared random, but the deviations increased with pressure. In the final inversion, the effect of these heteroscedastic random errors on the parameter estimation was further assessed. To stabilize the errors and make the data more normal distribution-like, the Box-Cox transformation (Box and Cox, 1964), which is a family of power transformations and alleviates heteroscedasticity in the error, was applied to the measured and simulated data.

The heterogeneity in the Box-Cox transformed residuals was significantly alleviated (see Fig. 5d), but in this monitoring scenario, this attempt did not necessarily improve the accuracy of the parameter estimation.

## CONCLUDING REMARKS

Detection of CO<sub>2</sub> or brine leakage depends on the sensitivity of system responses (monitoring data) to leakage pathways. Our study shows that pressure-based monitoring data are sensitive to leakage pathway properties and change with time and space, therefore allowing parameter estimation through inversion. While large random or systematic errors commonly occur in both the model and the data which can lead to biased parameter estimates, the parameterization of some of these errors in the inverse model greatly helps in mitigating the misfit between the observed and calculated system responses, and improves the estimation process.

In contrast to modeling with the simplified geometric conditions in our model, finding the sources of systematic or non-Gaussian errors may not always be possible for most practical cases. However, a detailed residual analysis on multiple complementary data might enable the modeler to identify such errors. More details on the error-handling strategies and capabilities for mitigating the impact of systematic or non-Gaussian random errors, particularly using iTOUGH2, can be found in Finsterle and Zhang (2011).



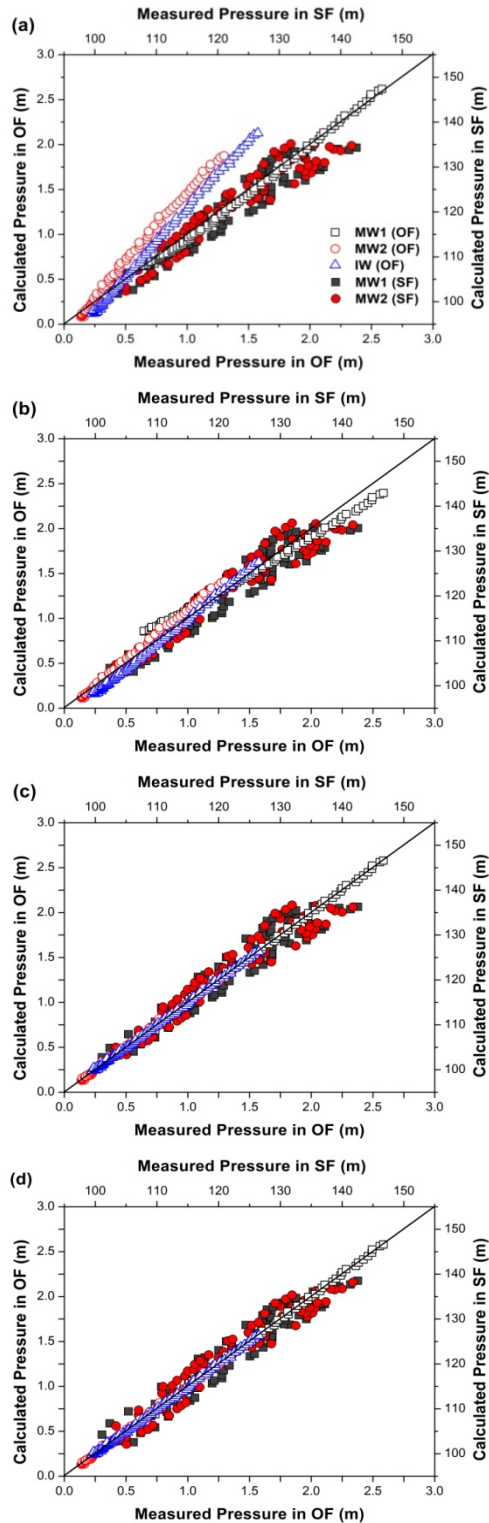


Figure 5. Measured vs. calculated pressures in the cases where (b)  $k'$ , (c) drift, and (d) Box-Cox parameter are incrementally included in the parameters calibrated, in addition to (a) the case with only the location and permeability of the leaky well calibrated. The solid line is the unit-slope line.

Table 2. Estimated parameters for inversion with different error handling.

Parameter	True	Inversion 1	Inversion 2	Inversion 3	Inversion 4
X [m]	2000	1499 ( $\pm 1031$ )*	1507 ( $\pm 201$ )	2212 ( $\pm 209$ )	2206 ( $\pm 256$ )
Y [m]	0	1501 ( $\pm 969$ )	1504 ( $\pm 222$ )	-11 ( $\pm 49$ )	-30 ( $\pm 109$ )
$\log(k_L \text{ [m}^2\text{)])}$	-10.0	-10.41 ( $\pm 0.08$ )	-10.18 ( $\pm 0.03$ )	-9.94 ( $\pm 0.06$ )	-9.94 ( $\pm 0.08$ )
$\log(k' \text{ [m}^2\text{)])}$	-18.0	n/a	-17.98 ( $\pm 0.003$ )	-18.01 ( $\pm 0.002$ )	-18.01 ( $\pm 0.002$ )
Drift [m d <sup>-1</sup> ]	0.001	n/a	n/a	9.82E-4 ( $\pm 1.76\text{E-}5$ )	9.85E-4 ( $\pm 1.67\text{E-}5$ )
Box-Cox [-]	n/a	n/a	n/a	n/a	-2.4 ( $\pm 7.37\text{E-}1$ )

\* Values in parentheses are the marginal standard deviation of the estimated parameter.

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